Supplementary Material

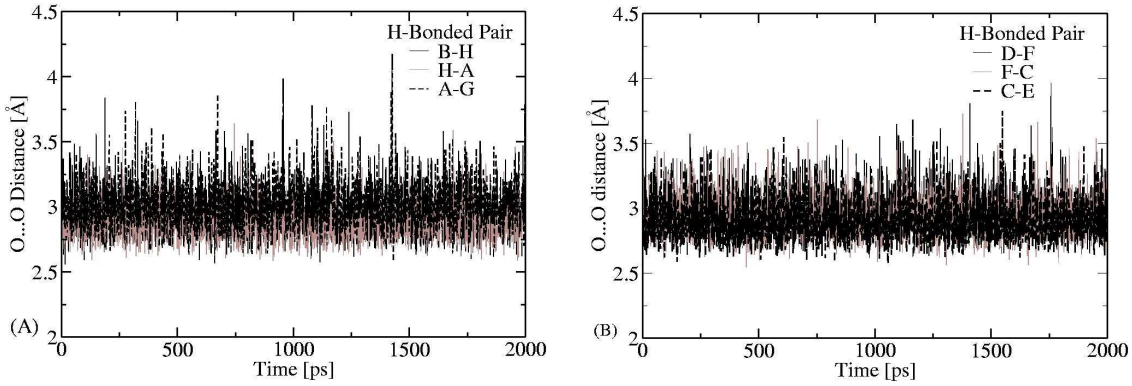

Figure 1: Time series of the hydrogen bond distances between two oxygen atoms that form a hydrogen-bonded pair (A) in the first chain between molecules B-H, H-A, A-G and (B) in the second chain between molecules D-F, F-C, C-E.

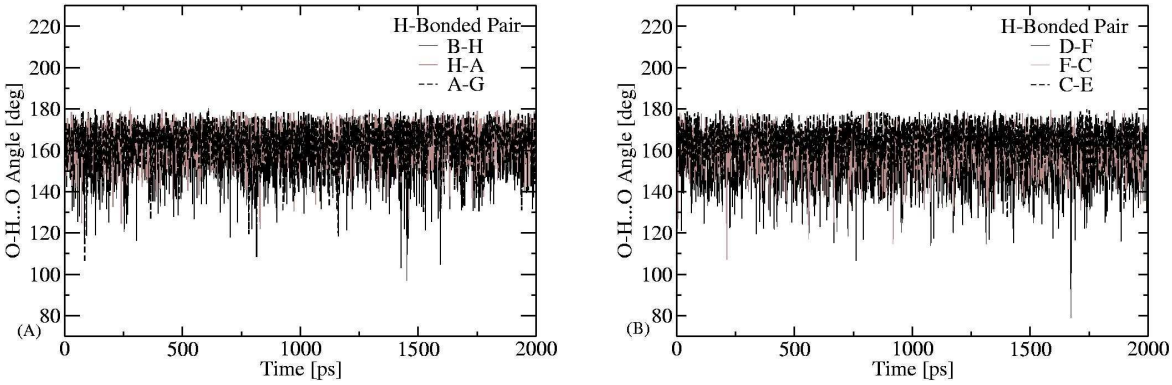

Figure 2: Time series of the hydrogen bond angles O-H...O between atoms that form a hydrogen-bonded pair (A) in the first chain between molecules B-H, H-A, A-G and (B) in the second chain between molecules D-F, F-C, C-E.

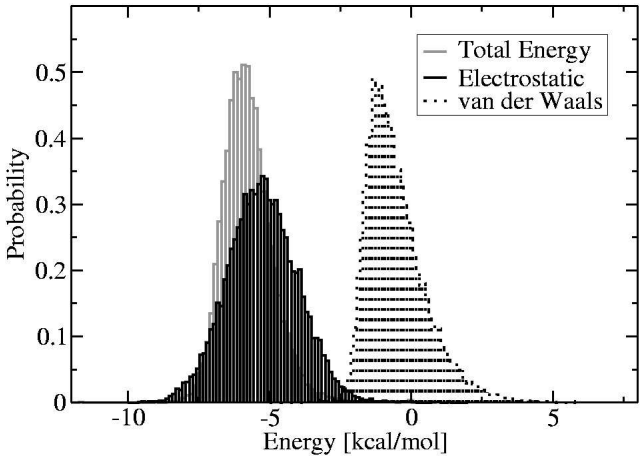

Figure 3: The total, van der Waals and electrostatic energy probability distributions for the hydrogen-bonded pair B–H. The main contribution to the interaction energy of a hydrogen bond arises from electrostatics.

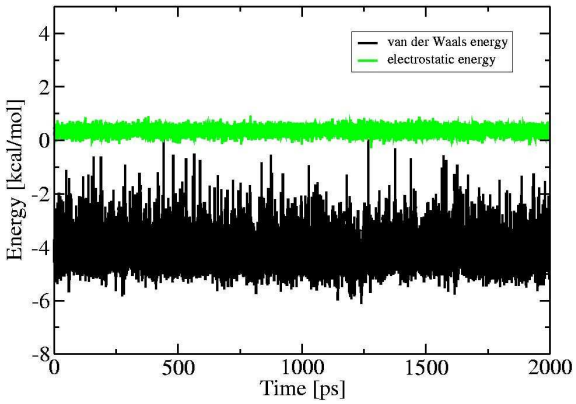

Figure 4: Time series of the van der Waals and electrostatic contributions to the total interaction energy between adjacent, along the a-axis, molecules B and D in the primary unit cell.

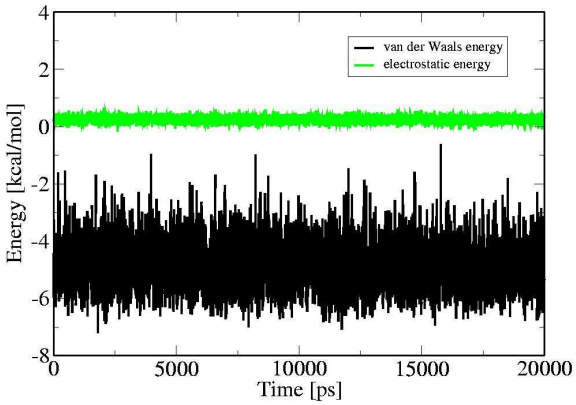

Figure 5: Time series of the van der Waals and electrostatic contributions to the total interaction energy between adjacent, along the a-axis, molecules C of the primary unit cell and molecule G of the neighboring cell.